

1,4-Benzoquinone
106-51-4 | DTXSID6020145

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 93.8 °C

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

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1,4-Benzoquinone

Measured: 116

Predicted: 93.8

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2-Methyl-p-benzoquinone

Measured: 69.0

Predicted: 72.7

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2,3-Dimethyl-2,5-cyclohexadiene-1,4 dione

Measured: 55.0

Predicted: 67.2

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2,6-Dimethyl-1,4-benzoquinone

Measured: 72.5

Predicted: 67.2

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Coumaranone

Measured: 103

Predicted: 89.0